Congressional Notification Profile
DE-PS26-02NT41369

UNIVERSITY COAL RESEARCH PROGRAM, INNOVATIVE CONCEPTS PROGRAM

Duquesne University

Background and Technical Information:

Project Title: "Use of Molecular Modeling to Determine the Interaction and Competition of Gases Within Coal for Carbon Dioxide Sequestration."

Duquesne University will generate a 3-dimensional, state-of-the-art molecular model of a low-volatile bituminous coal that may lead to low-cost methods of sequestering carbon dioxide. By using the model to uncover interactions between small molecules and simple aromatic structures, the university will apply the data to enhance the CO_2 sequestration from the combustion of more complex coal structures. This approach will also address coalbed methane issues and contribute to the understanding of greenhouse gases.

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Congressional District: PA 14th County: Allegheny

Financial Information:

Length of Contract (months): 36-60
Government Share: $200,000
Total value of contract: $200,000

DOE Funding Breakdown:

Funds: FY 2002 $200,000

Public Abstract
Use of Molecular Modeling to Determine the Interaction and Competition of Gases Within Coal for Carbon Dioxide Sequestration

The objective is to generate a realistic and testable three-dimensional state-of-the-art molecular model of a low volatile bituminous coal to assist in the optimization of CO2 sequestration. The plan is to uncover the fundamental and physical interactions between small molecules and simple aromatic structures in confined nanospaces, and use the computed information to enhance the sequestration of CO2 in more complex coal structures. Density functional theory, second-order Moller-Plesset theory, and classical molecular dynamics will be used to investigate three chemical models of coal.

In order of increasing model sophistication, small molecules (CH4, CO2, and N2) will be studied with (a) anthracene, (b) nanotube(s), and (c) models of bituminous coal structure. The quantum chemical information will be used to calibrate and parameterize the force field for the molecular dynamics simulations. The use of large-scale molecular dynamics simulations (> 50,000 atoms) will be used to follow the molecular interactions between gases and the coal matrix. The proposed molecular simulations will provide useful information that includes: accessible pore volumes, energy of interactions between host and guest molecules, self-diffusion coefficients, identification of likely sorption sites, impact of carbon dioxide sorption/methane exchange upon the coal matrix (expansion/contraction), and competitive adsorption isotherms.

The computed atomic-level structural and dynamical information will aid in the optimal geological sequestration of CO2. The proposed use of molecular simulations upon a realistic molecular model of coal is an innovative research approach that until recently was not a viable procedure. The implementation of such a plan is now possible through the combination of recent experimental advances in coal structural elucidation and diversity, and significant increases in computer hardware and simulation methodologies.

The merger of coal science experts from Penn State University with the computational expertise and large-scale computer facilities at Duquesne University represents a unique and powerful opportunity to advance the necessary technology to sequester CO2.

The use of the coal model and simulation results may also prove useful in many other areas of coal science, such as chemical changes during combustion, constitutional changes during maturation, solvent swelling, solvent extraction, liquefaction, coal bed methane production, pollutant formation during combustion, and gasification. This novel computational approach, which couples computed structural and dynamic atomic-level information with observed experimental data, has the potential to contribute significantly to the base of knowledge required to address the technological problem of CO2 sequestration. New opportunities in the optimization and gaseous management necessary for low-cost forms of CO2 sequestration will result from this novel procedure.